



# A multi-scale thermal model of a high-power LiFePO<sub>4</sub> lithium-ion cell

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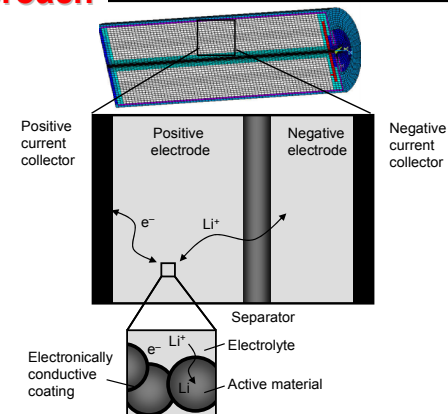
## Introduction and goals

- Battery performance and lifetime are influenced by temperature
- Risk of fire and explosion at high  $T$
- Thermal stability vital for safety and cost
- Thermal modeling is an effective tool for predicting cell thermal behavior
- A complete thermal model consists of a heat generation model and a heat transport model
- Goal: Study the temperature and heat flow patterns of a LiFePO<sub>4</sub>-based cell under variable loads



## Multi-scale approach

- A multi-scale thermal model for a LiFePO<sub>4</sub> lithium-ion cell is developed
- Heat transport in single cell: ~ 20 mm scale
- Li<sup>+</sup> charge transport in electrolyte: ~ 100  $\mu$ m scale
- Li transport in solid phase: ~ 100–1000 nm scale



## Model equations

### Electrochemical model

#### Thermodynamics

$$\Delta\phi_{eq}(c_{Li}) = \frac{\Delta G}{zF} = \frac{\Delta H(c_{Li}) - T\Delta S(c_{Li})}{zF}$$

#### Kinetics

$$i = i_0 \left( \exp\left(\frac{\alpha F}{RT} \eta_{act}\right) - \exp\left(-\frac{(1-\alpha)F}{RT} \eta_{act}\right) \right)$$

$$\eta_{conc} = \frac{RT}{zF} \ln\left(\frac{c_0}{c(t)}\right) \quad \eta_{act} = \Delta\phi(t) - \Delta\phi_{eq}(c_{Li}) - \eta_{conc}$$

#### Solid-state transport

$$\frac{\partial c_{Li}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D \frac{\partial c_{Li}}{\partial r} \right) - \frac{M_{Li}}{zF} i$$

#### Electrolyte transport

$$\frac{\partial(c_{Li})}{\partial t} = \frac{\partial}{\partial y} \left( D_e \frac{\partial c_{Li}}{\partial y} \right) + \frac{zF}{RT} \frac{\partial}{\partial y} \left( D_e c_{Li} \frac{\partial \phi}{\partial y} \right) + M_e s_y'$$

$$\sum (c_{Li}) = 0$$

#### Heat Generation $Q_{total} = Q_{elchem} + Q_{ohm}$

### Heat transfer model

- 3D finite element model using ANSYS

#### Heat transfer inside the cell

$$\rho C_{p,cell} \frac{\partial T_{cell}}{\partial t} = \nabla \cdot (\lambda_{cell} \nabla T_{cell}) + Q_{total}$$

#### Heat transfer out of the Cell

$$Q_{total} = h_f A (T_{cell} - T_{env})$$

#### Assumptions:

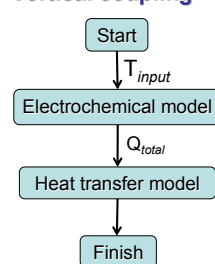
- Jellyroll modeled as a single material with distinct thermal properties
- Variations in  $\theta$  direction ignored
- Effects of current collector perturbations ignored

**Parameters:** Thermal conductivity and heat capacity were determined experimentally

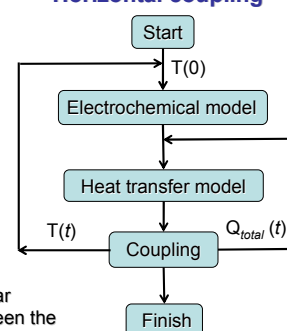
## Multi-scale simulation

- Vertical (indirect) and horizontal (direct) coupling used for interaction

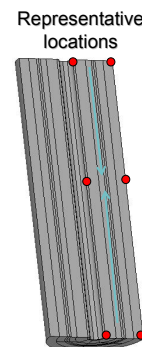
### Vertical coupling



### Horizontal coupling

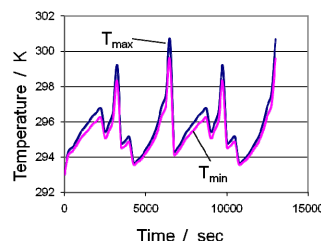
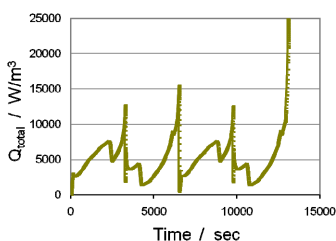


- In horizontal coupling linear interpolation is used between the representative points

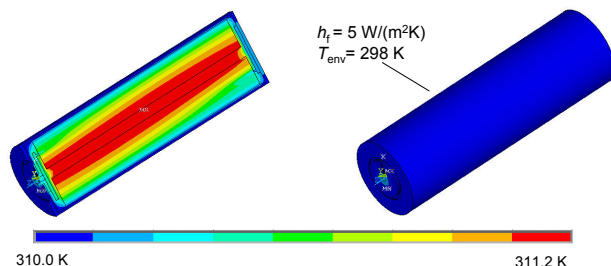


## Simulation results

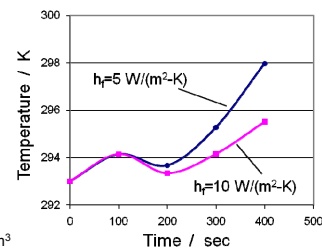
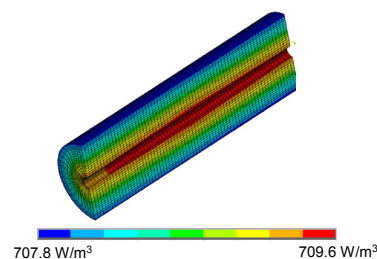
### Vertical (indirect) multi-scale coupling



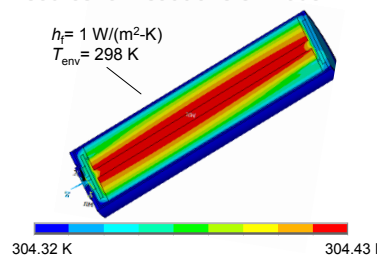
- Heat generation obtained from electrochemical simulation used as input load for heat transfer model
- Temperature distribution inside and outside the cell
- Minimum and maximum temperature profiles obtained from heat transfer simulations



### Horizontal (direct) multi-scale coupling



- Linearly interpolated contours of heat generation from electrochemistry model used as input heat source for heat transfer model
- An example simulation result showing surface temperature versus time at 5C-rate using two different boundary conditions with  $T_{env} = 298$  K
- An example simulation result showing temperature distribution over half cell geometry at 2C-rate



## Conclusions

- Model found to be useful in predicting thermal behavior of the cell under variable loads
- Small gradient of temperature was observed in axial direction as compared to the radial direction

## Future work

- Improve parameterization of model
- Validation of the model with experimental findings
- Expand the model to be used with variable boundary conditions
- Expand the model to module level